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The funds awarded were used to purchase an eight node IBM J50 computer, and the associated software. Each node is configured with 256MB of memory and 4 GB of disk. The system is currently being run as eight separate nodes. In addition to the DoD funds, IBM provided $40,000 in matching funds for this project. The IBM funds were used to purchase two dual processor 233 MHz IBM 43P computers. These are PCI-based systems, each of which is configured with 512 MB of memory and 9 GB of disk. As for the J50, we are using these systems as two independent nodes, until the parallel environment is released. Finally, Apple Computer has given us a high end Macintosh computer as part of their match. This computer has already played a central role in the development of MacMolPlt, a graphical interface for our electronic structure code GAMESS.

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FINAL TECHNICAL REPORT
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The funds awarded were used to purchase an eight node IBM J50 computer, and the associated software. Each node is configured with 256MB of memory and 4 GB of disk. The system is currently being run as eight separate nodes, because IBM has been slower than expected in releasing the parallel software necessary to effectively run a J50 as a shared memory parallel (SMP) computer. We now have assurance from IBM that the parallel environment will be forthcoming within the next few months. We will then begin to evaluate the performance of the system in an SMP environment.

In addition to the DoD funds, IBM provided $40,000 in matching funds for this project. The IBM funds were used to purchase two dual processor 233 MHz IBM 43P computers. These are PCI-based systems, each of which is configured with 512 MB of memory and 9 GB of disk. As for the J50, we are using these systems as two independent nodes, until the parallel environment is released. Finally, Apple Computer has given us a high end Macintosh computer as part of their match. This computer has already played a central role in the development of MacMolPlt, a graphical interface for our electronic structure code GAMESS. The Mac has been used by Brett Bode to develop several new features for MacMolPlt, including the ability to plot atomic and molecular orbitals, electron densities, density differences, and electrostatic potential maps in 2-D or 3-D. One can also make these plots at several points along a reaction path, and animate the sequence, so that one can visualize the changes in bonding as a reaction proceeds. Another new feature in MacMolPlt is its ability to generate input files for GAMESS. This makes perparation or modification of input files much easier.

The IBM computers are being used for a variety of AFOSR-related research projects. These include:

1. The investigation of potential high energy fuels. Galina Chaban has been examining the behavior of Al-doped matrices of molecular hydrogen, in order to determine that stability of such species, and to determine how easily an Al atom can migrate in the lattice. This is important, since two Al atoms would immediately for a diatomic molecule if they could find each other, and this would greatly reduce the utility of the system as a fuel. A closely related project being studied by Michael Pak is the analysis of the potential energy surface for these Al atoms reacting with molecular oxygen. This should provide some important insight regarding the identity and the mechanism of formation of the Al oxides that are formed when such a fuel is burned. There has been considerable interest in other groups in heterocubanes, including N8. Mike Schmidt has extensively studied the N8 potential energy surface and shown that the upper limit to the barrier for decomposition of this molecule to four N2's is only 20 kcal/mol. So, N8 may not be a viable fuel.

2. Design of new materials. Brett Bode is extensively studying the effect of catalysts (modeled by divalent titanium) on the hydrosilation reaction, in which a silane reacts with an alkene to form a new SiC bond. Such species are important, because they are precursors to silicon carbide. Brett has shown that the origin of the catalytic activity for TiR2 is its ability to form an extremely stable complex with ethylene. The excess energy due to the formation of this complex is sufficient to overcome all subsequent barriers in the mechanism. Takako Kudo is studying the mechanisms for formation of polyhedral oligomeric silsesquioxanes (POSS). These species are of considerable interest to the Air Force because of their potential use as lubricants and as materials precursors. This

investigation will examine the effects of solvent, substitutents, and catalysts on the POSS formation mechanism. Vanda Glezakou is examining the mechanism of formation of metallocarbohedrenes (met-cars), an unusually stable TiC analog of C20. The interest in these species is as potential nanostructural materials. They are apparently formed by the laser ablation of titanium in the presence of alkanes and alkenes, so Vanda is studying the reactions of Atomic Ti with small alkenes.